Coherent Scattering of Strained Nanocrystals

Weijie Huang, R.S. Sun, *J.M. Zuo*

Department of Materials Science and Engineering, University of Illinois Urbana-Champaign, 1304 W Green Street, Urbana, IL 61801

Atoms on surfaces adopt different bond lengths because of redistribution of bonding electrons. The strain induced by surface atom reconstruction can have a large effect on nanocrystal properties. Coherent scattering can be used to probe strain field in nanocrystals as demonstrated by Robinson's group recently. Here we show that the technique can be extended to study surface strain in nanocrystals of a few nanometers in diameter using coherent electron diffraction. The experimental was carried for Au nanocrystals of 3 to 6 nm in diameter. By measuring the asymmetry in the intensity oscillations around the Bragg spots, we show the surface strain can be determined including the direction of the dominant strain. Furthermore, we modeled the coherent scattering using nanocrystal models generated by molecular dynamics simulations and bond lengths from Linus Pauling. We show that there is a good agreement between the experimental coherent scatterings and these obtained from the MD simulations. Experimental patterns and the MD results suggest that the contraction of surface atoms is surface dependent: the surface strain of the Au nanocrystal is dominated by the strain of the (100) surfaces. The present work shows the potential of coherent scattering for probing three-dimensional surfaces of nanocrystals.